

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063023\
 Data File : BF134052.D
 Acq On : 30 Jun 2023 14:46
 Operator : CG\JU
 Sample : PB153881BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB153881BL

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134052.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.504	407	411	420	rBV	354820	393773	7.85%	1.269%
2	5.116	508	515	527	rBV	1319120	1933775	38.54%	6.233%
3	5.504	575	581	584	rBV	3410564	3611378	71.97%	11.640%
4	6.492	743	749	752	rBV	3148436	3627015	72.28%	11.690%
5	6.845	806	809	816	rBV	883227	764535	15.24%	2.464%
6	7.416	899	906	909	rBV	2350606	2419625	48.22%	7.799%
7	7.845	974	979	989	rBV	37375	53577	1.07%	0.173%
8	8.128	1021	1027	1030	rBV	1280812	1020429	20.34%	3.289%
9	9.210	1204	1211	1214	rBV	4851705	4435516	88.39%	14.296%
10	9.886	1322	1326	1330	rBV	1385454	1147174	22.86%	3.697%
11	10.686	1456	1462	1465	rBV	3253625	3161679	63.01%	10.190%
12	11.380	1576	1580	1588	rBV	1412830	1289460	25.70%	4.156%
13	12.986	1847	1853	1856	rBV	4843020	5018005	100.00%	16.173%
14	14.039	2028	2032	2040	rBV	1119177	1118982	22.30%	3.607%
15	14.310	2068	2078	2087	rBV6	28368	132481	2.64%	0.427%
16	15.545	2283	2288	2293	rBV	640531	898797	17.91%	2.897%

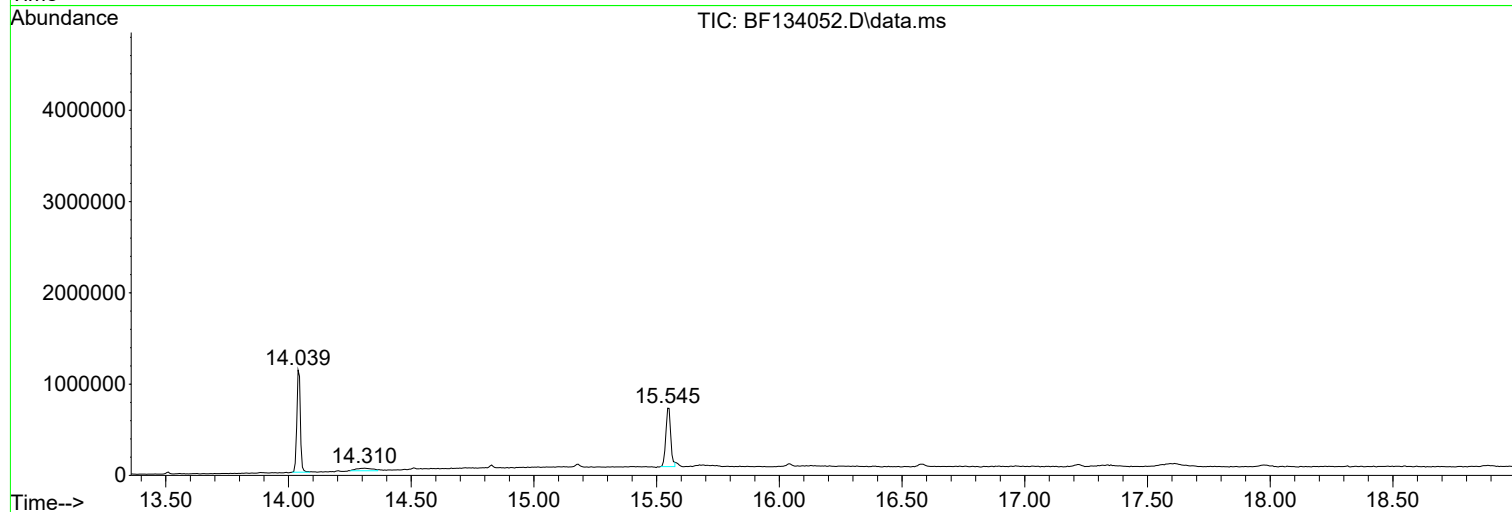
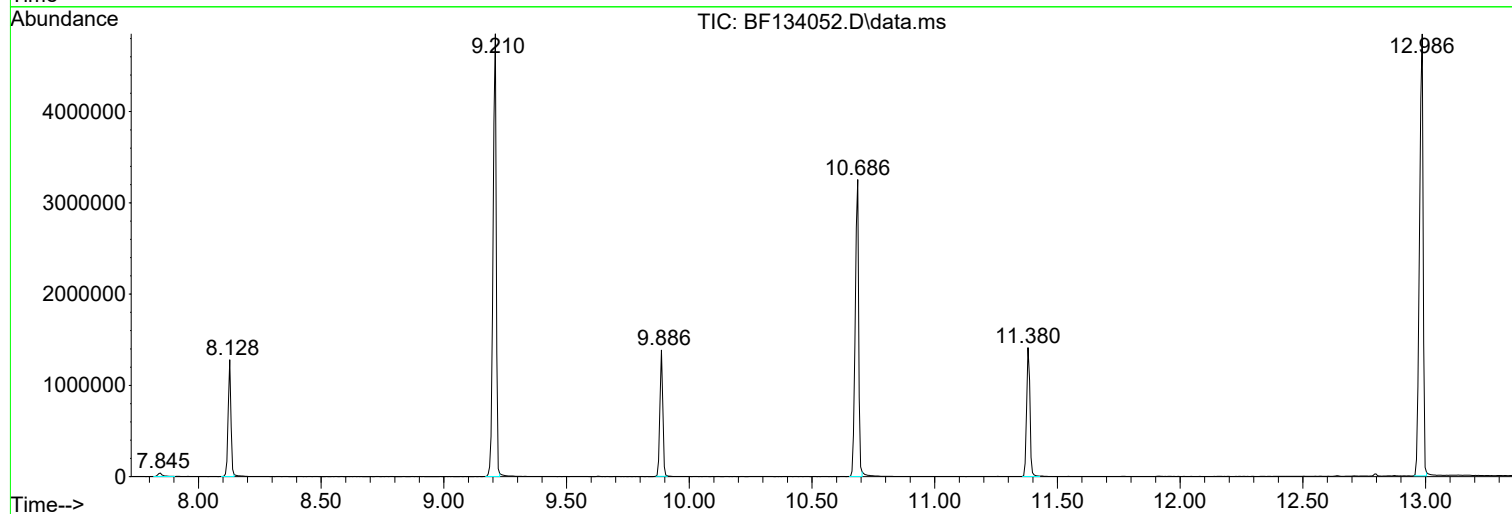
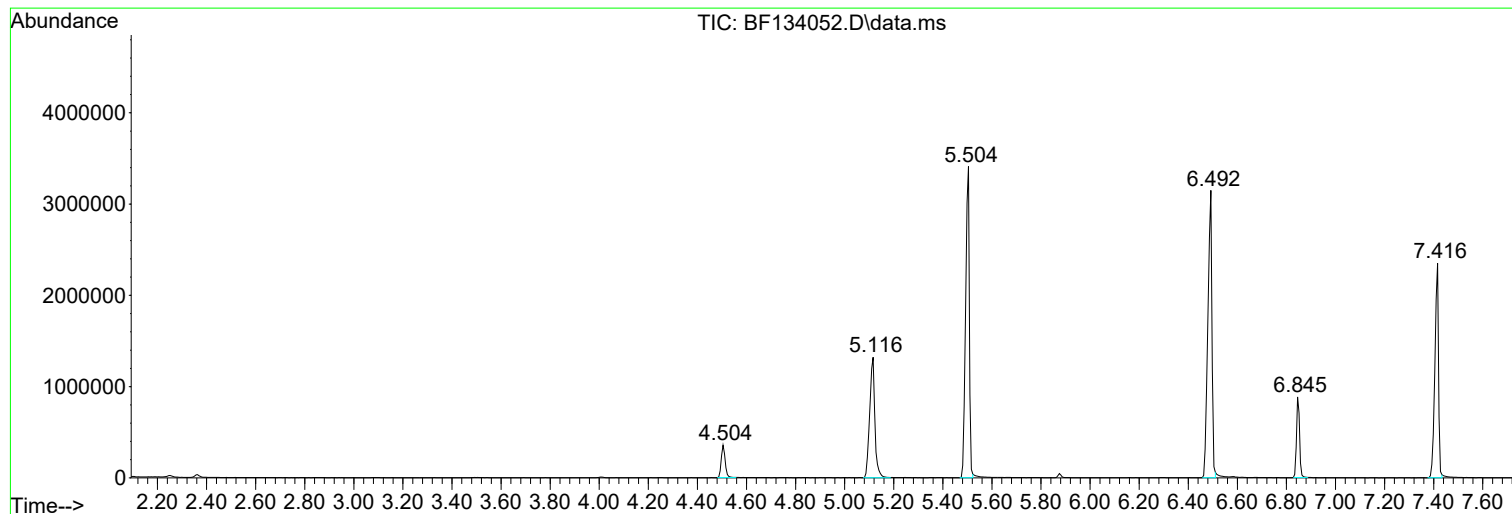
Sum of corrected areas: 31026201

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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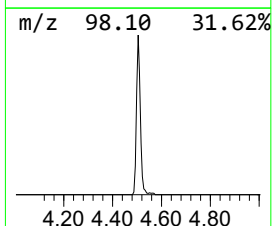
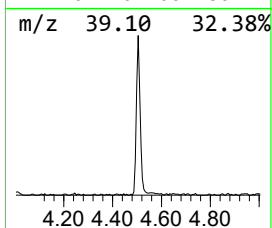
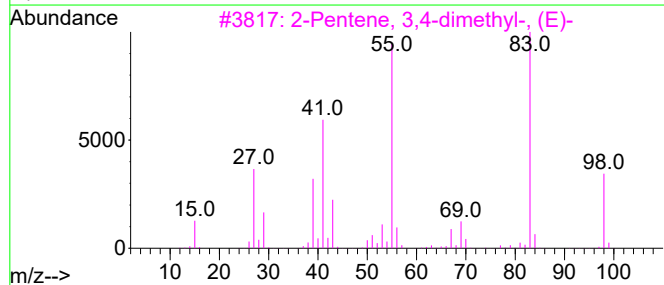
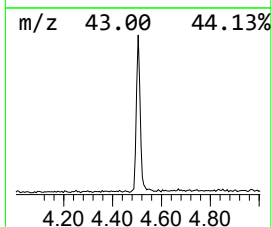
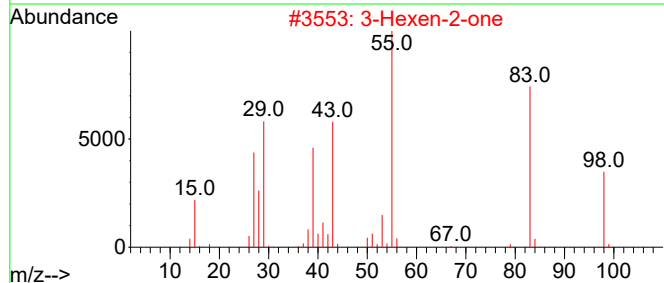
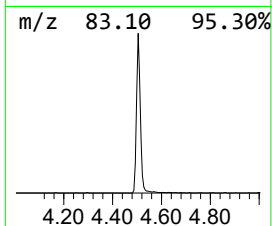
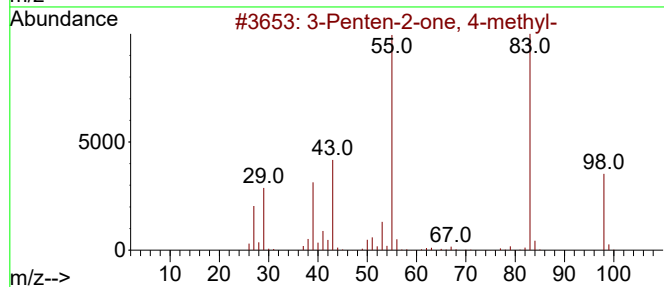
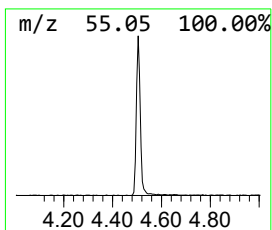
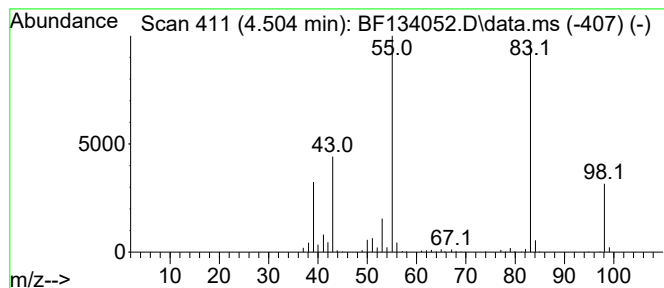
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.504	10.30 ng	393773	1,4-Dichlorobenzene-d4	6.845

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86



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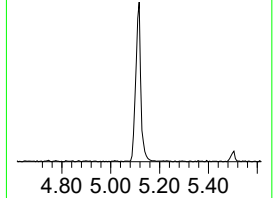
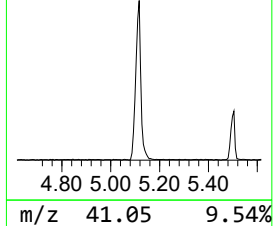
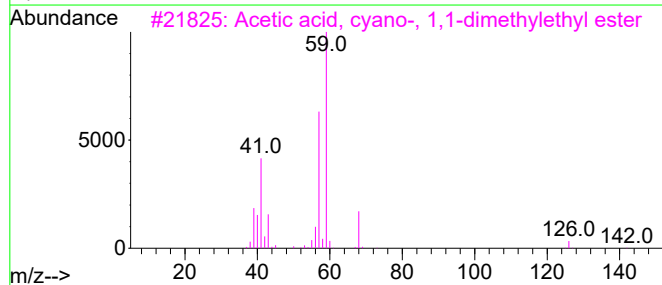
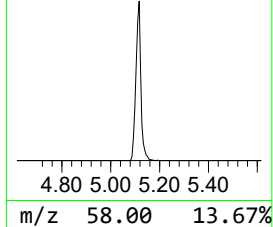
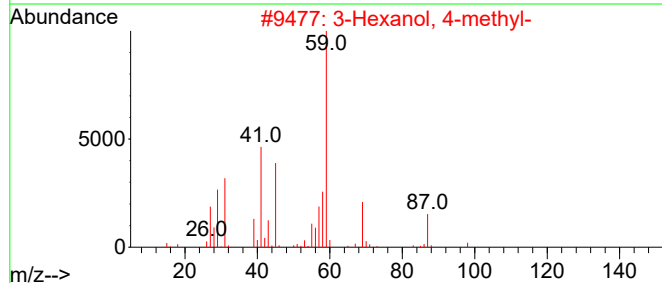
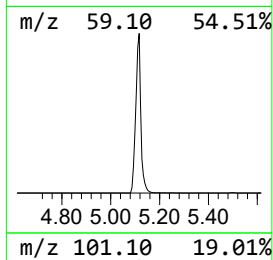
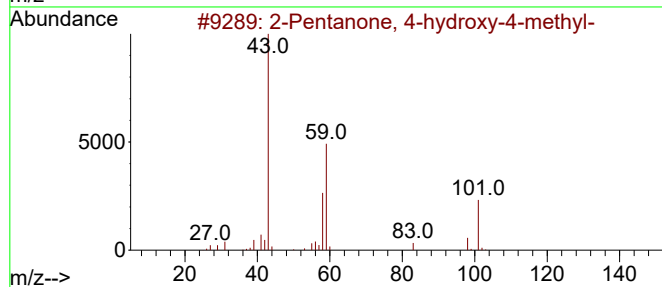
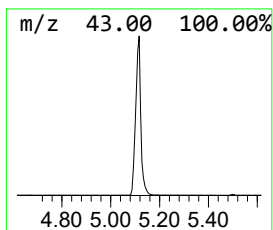
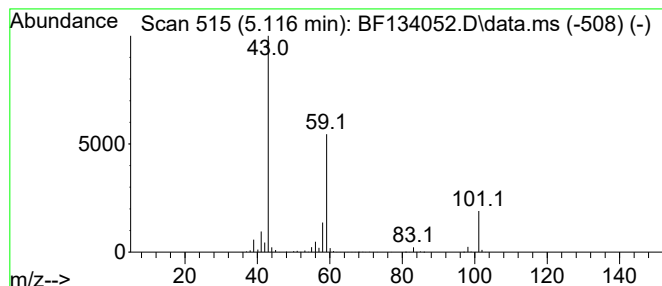
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.116	50.59 ng	1933780	1,4-Dichlorobenzene-d4			6.845
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	12
5	Morpholine, 4-methyl-		101	C5H11NO	000109-02-4	9



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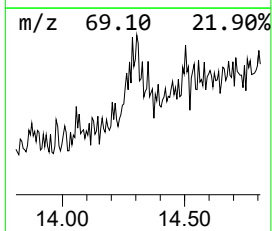
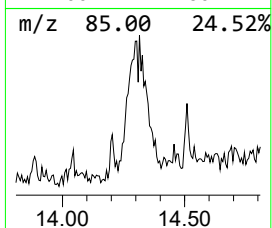
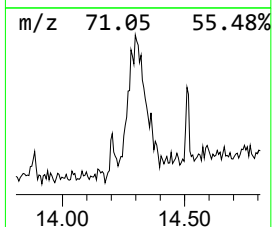
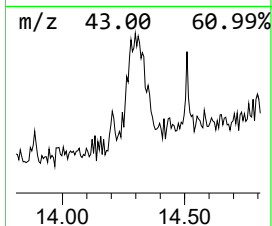
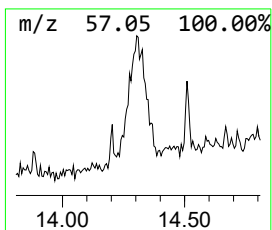
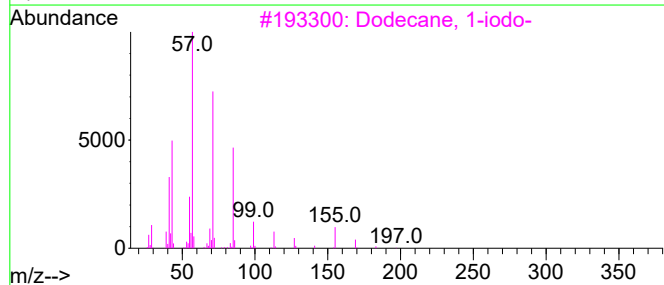
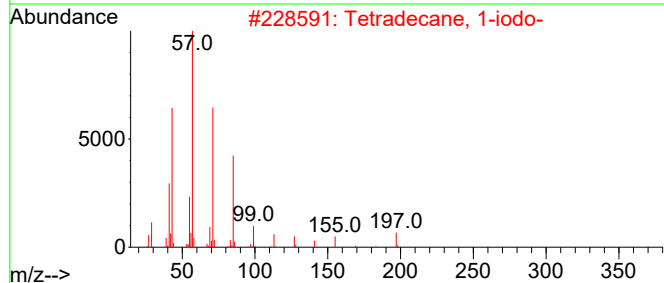
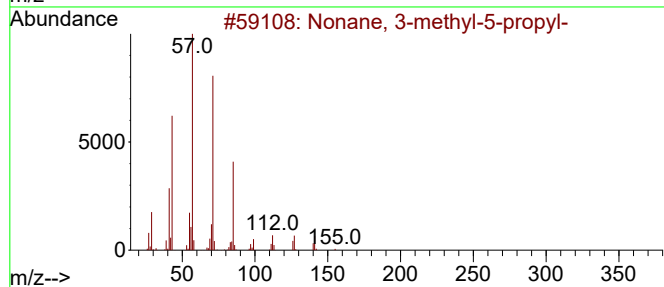
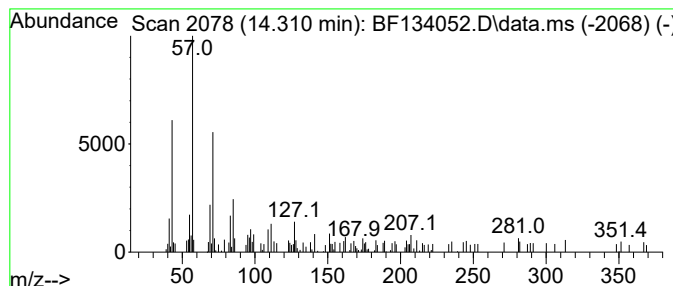
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Peak Number 3 unknown14.310 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.310	2.37 ng	132481	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	47
2			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	47
3			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	47
4			Heptacosane	380	C27H56	000593-49-7	47
5			Tetradecane, 4-methyl-	212	C15H32	025117-24-2	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.504	10.3	ng	393773	1	6.845	764535	20.0
2-Pentanone, 4-...	5.116	50.6	ng	1933780	1	6.845	764535	20.0
unknown14.310	14.310	2.4	ng	132481	5	14.039	1118980	20.0